Confined active matter in external fields
Supplementary information

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I. ANALYTICAL EXPRESSIONS FOR THE NUMBER DENSITY AND THE POLAR ORDER

Here we give full analytical expressions for the number density and polar order fields referred to in the main text. The variables have been non-dimensionalized using the rotational diffusion time τ_R, the run length ℓ, and the speed in the absence of fields U_0 (note L here is dimensionless, representing L/ℓ in dimensional form).

For active matter confined between walls at $x = 0$ and L, we find the number density and polar order by solving Eqs. (2), (3) in the main text along with the constraints $\mathbf{n} \cdot \mathbf{j}_n|_{\text{wall}} = 0$ and $\mathbf{n} \cdot \mathbf{j}_m|_{\text{wall}} = \mathbf{0}$. We solve these equations asymptotically by doing a singular perturbation expansion in Pe^{-1} for $\text{Pe}L \gg 1$. Additionally, in the absence of external field, an exact solution valid at any $\text{Pe}L$ is also found. In either case, the aforementioned no-flux conditions determine solutions up to a multiplicative constant that is found using the additional constraint $\frac{1}{L}\int_0^L n\,dx = \langle n \rangle = \frac{1}{L}$.

When there is no external field ($U = 1$, $\chi_R = 0$), the exact solution is

$$\frac{n}{n_c} = \gamma b \left[\cosh\left(\lambda\left(x - \frac{L}{2}\right)\right) - 1\right] + 1, \tag{1}$$

$$\frac{m_x}{n_c} = b \sinh\left(\lambda\left(x - \frac{L}{2}\right)\right), \tag{2}$$

where

$$b = \frac{\gamma}{d\left\{1 + \Lambda\left[\cosh\left(\frac{\lambda L}{2}\right) - 1\right]\right\}}, \tag{3}$$

$$\lambda = \text{Pe}\sqrt{\frac{1}{d} + \frac{(d-1)}{\text{Pe}}},\ \Lambda = \frac{1}{1 + \frac{\text{Pe}}{d(d-1)}},\ \gamma = \sqrt{\frac{d}{1 + \frac{d(d-1)}{\text{Pe}}}}. \tag{4}$$

Here, n_c is the number density at the center of the confinement and can be found using the constraint $\frac{1}{L}\int_0^L n\,dx = \langle n \rangle$. This exact solution is consistent with the previous calculation on confined active matter [1]. The number density in (1) rewritten as

$$\frac{n}{n_0} = 1 + \frac{\text{Pe}}{d\,(d-1)} \frac{\sinh(\lambda x) + \sinh(\lambda (L - x))}{\sinh(\lambda L)} \tag{5}$$

where $n_0 = \frac{n_c}{1 + \frac{\text{Pe}}{d(d-1)}\frac{1}{\cosh(\lambda L/2)}}$, is similar to that reported in Ref. [2].

The exact solution expanded in Pe^{-1} takes the form

$$\frac{n}{n^{bulk}} = 1 + \frac{\text{Pe}}{d\,(d-1)}\left\{e^{-\lambda x} + e^{-\lambda(L-x)}\right\} + O\left(\text{Pe}^{-1}\right), \tag{6}$$

$$\frac{m_x}{n^{bulk}} = \frac{\lambda}{d\,(d-1)}\left\{-e^{-\lambda x} + e^{-\lambda(L-x)}\right\} + O\left(\text{Pe}^{-1}\right) \tag{7}$$

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where the bulk number density $n^{bulk} = n_c$. Here, the leading order terms display a linear combination of the near-wall solution [2] and the bulk solution.

In the presence of a field that modulates the self-propulsion speed in the wall normal direction (say $U = 1 - \alpha_L\left(\frac{x}{L} - \frac{1}{2}\right)$), the asymptotic solution for weak fields ($\alpha_L \ll 1$) is

$$\frac{n}{n_c} = \frac{1}{U} + \frac{\mathrm{Pe}}{d\,(d-1)}\left\{U_l e^{-\lambda_l x} + U_r e^{-\lambda_r (L-x)}\right\} + O\left(\mathrm{Pe}^{-1}, \frac{\alpha_L}{\mathrm{Pe}L}\right), \tag{8}$$

$$\frac{m_x}{n_c} = \frac{1}{d\,(d-1)}\left\{-\lambda_l e^{-\lambda_l x} + \lambda_r e^{-\lambda_r (L-x)}\right\} + O\left(\mathrm{Pe}^{-1}, \frac{\alpha_L}{\mathrm{Pe}L}\right). \tag{9}$$

Here, $U_l = 1 + \frac{\alpha_L}{2}$ and $\lambda_l = \mathrm{Pe}\sqrt{\frac{U_l^2}{d} + \frac{(d-1)}{\mathrm{Pe}}}$ are the speed and the inverse boundary layer thickness at the left wall. The corresponding quantities at the right wall are $U_r = 1 - \frac{\alpha_L}{2}$ and $\lambda_r = \mathrm{Pe}\sqrt{\frac{U_r^2}{d} + \frac{(d-1)}{\mathrm{Pe}}}$.

On the other hand, in the presence of a field that orients the particles normal to the walls and for field strengths $\chi_R \ll \lambda \sim \mathrm{Pe}$, the asymptotic solution expanded in terms of $\lambda^{-1} \sim \mathrm{Pe}^{-1}$ is

$$n = n^{(0)} + \frac{1}{\lambda}n^{(1)} + O\left(\mathrm{Pe}^{-2}, \frac{\chi_R}{\mathrm{Pe}^2}\right),\ m_x = m_x^{(0)} + \frac{1}{\lambda}m_x^{(1)} + O\left(\mathrm{Pe}^{-2}, \frac{\chi_R}{\mathrm{Pe}^2}\right). \tag{10}$$

Here, the leading order solution is

$$\frac{n^{(0)}}{n_c^{(0)}} = e^{\chi_R(d-1)(x-L/2)} + \frac{\mathrm{Pe}}{d\,(d-1)}\left\{e^{-\chi_R(d-1)L/2}e^{-\lambda x} + e^{\chi_R(d-1)L/2}e^{-\lambda(L-x)}\right\}, \tag{11}$$

$$\frac{m_x^{(0)}}{n_c^{(0)}} = \frac{\lambda}{d\,(d-1)}\left\{-e^{-\chi_R(d-1)L/2}e^{-\lambda x} + e^{\chi_R(d-1)L/2}e^{-\lambda(L-x)}\right\} \tag{12}$$

while the first order solution is

$$\begin{aligned} n^{(1)} = {} & e^{-\chi_R(d-1)L/2}e^{-\lambda x}\left\{\begin{array}{l} -\dfrac{\chi_R \mathrm{Pe}^3 n_c^{(0)}}{2\lambda d^2}x \\ +\dfrac{\mathrm{Pe}}{d\,(d-1)}\left(n_c^{(1)} + \dfrac{\chi_R\lambda L d(d-1)^2 n_c^{(0)}}{2\mathrm{Pe}} - \dfrac{\chi_R \mathrm{Pe} n_c^{(0)}}{d}\right)\end{array}\right\} \\ & + e^{\chi_R(d-1)\left(x-\frac{L}{2}\right)}\left(n_c^{(1)} - \frac{\chi_R\lambda d(d-1)^2 n_c^{(0)}}{\mathrm{Pe}}\left(x - \frac{L}{2}\right)\right) \\ & + e^{\chi_R(d-1)L/2}e^{-\lambda(L-x)}\left\{\begin{array}{l} \dfrac{\chi_R \mathrm{Pe}^3 n_c^{(0)}}{2\lambda d^2}(L-x) \\ +\dfrac{\mathrm{Pe}}{d\,(d-1)}\left(n_c^{(1)} - \dfrac{\chi_R\lambda L d(d-1)^2 n_c^{(0)}}{2\mathrm{Pe}} + \dfrac{\chi_R \mathrm{Pe} n_c^{(0)}}{d}\right)\end{array}\right\}, \end{aligned} \tag{13}$$

$$\begin{aligned} m_x^{(1)} = {} & e^{-\chi_R(d-1)L/2}e^{-\lambda x}\left\{\begin{array}{l} \dfrac{\chi_R \mathrm{Pe}^2 n_c^{(0)}}{2d^2\lambda}(\lambda x - 1) \\ -\dfrac{\lambda}{d\,(d-1)}\left(n_c^{(1)} + \dfrac{\chi_R\lambda L d(d-1)^2 n_c^{(0)}}{2\mathrm{Pe}} - \dfrac{\chi_R \mathrm{Pe} n_c^{(0)}}{d}\right)\end{array}\right\} \\ & + \frac{\chi_R\lambda\,(d-1)\,n_c^{(0)}}{\mathrm{Pe}}e^{\chi_R(d-1)\left(x-\frac{L}{2}\right)} \\ & + e^{\chi_R(d-1)L/2}e^{-\lambda(L-x)}\left\{\begin{array}{l} \dfrac{\chi_R \mathrm{Pe}^2 n_c^{(0)}}{2d^2\lambda}(\lambda(L-x) - 1) \\ +\dfrac{\lambda}{d\,(d-1)}\left(n_c^{(1)} - \dfrac{\chi_R\lambda L d(d-1)^2 n_c^{(0)}}{2\mathrm{Pe}} + \dfrac{\chi_R \mathrm{Pe} n_c^{(0)}}{d}\right)\end{array}\right\}. \end{aligned} \tag{14}$$

The concentration at the center of the confinement at leading and first order, $n_c^{(0)}$, $n_c^{(1)}$, respectively, can be found from the constraints $\frac{1}{L}\int_0^L n^{(0)}dx = \langle n\rangle$ and $\int_0^L n^{(1)}dx = 0$. In addition to the constraint $\chi_R \ll \mathrm{Pe}$, we need also $\chi_R \leq O(1)$ for this theory to hold because otherwise the nematic order becomes large enough to invalidate the zero nematic order closure based on which this theory is built.

In the main text, we only considered the leading order solution to develop a simple theory. But the accuracy of this theory and hence the match with Brownian Dynamics (BD) simulations can be improved by considering the next order solution. For instance, the number density and polar order reported in Fig. 4 in the main text become those shown in Fig. S1 here, upon inclusion of the next order solution; the improvement in matching with the BD simulations is apparent.

If the orienting field in wall normal direction is not constant and varies spatially, $\mathbf{H} = H(x)\,\hat{\mathbf{H}}$, then the asymptotic solution for field strengths $\chi_R \ll \lambda \sim \mathrm{Pe}$ is

$$\frac{n}{n_c} = e^{-\chi_R(d-1)G(L/2)}\left\{\begin{array}{c} e^{\chi_R(d-1)G(x)} \\ +\,\dfrac{\mathrm{Pe}}{d(d-1)}\left(e^{\chi_R(d-1)G(0)}e^{-\lambda x} + e^{\chi_R(d-1)G(L)}e^{\lambda(x-L)}\right)\end{array}\right\} + O\left(\mathrm{Pe}^{-1}, \frac{\chi_R}{\mathrm{Pe}}\right), \tag{15}$$

$$\frac{m_x}{n_c} = \frac{\lambda e^{-\chi_R(d-1)G(L/2)}}{d(d-1)}\left\{-e^{\chi_R(d-1)G(0)}e^{-\lambda x} + e^{\chi_R(d-1)G(L)}e^{\lambda(x-L)}\right\} + O\left(\mathrm{Pe}^{-1}, \frac{\chi_R}{\mathrm{Pe}}\right). \tag{16}$$

Here, $G(x) = \int H(x)\,dx$ and the concentration at the center of the confinement n_c can again be found from the constraint $\frac{1}{L}\int_0^L n dx = \langle n\rangle$.

Lastly, in the presence of a field that orients particles parallel to the walls, the number density n and the polar order normal to the walls m_x are independent of the field and hence follow the expressions derived in the absence of field (6), (7). But the polar order along the walls m_y depends on the field and satisfies

$$\frac{m_y}{n^{bulk}} = \frac{\chi_R}{d} + \frac{\mathrm{Pe}^2\chi_R}{\left((d-1)\mathrm{Pe} - \lambda^2\right)d^2}\left\{e^{-\lambda x} + e^{-\lambda(L-x)}\right\} - \frac{\mathrm{Pe}^{3/2}\lambda\chi_R}{\left((d-1)\mathrm{Pe} - \lambda^2\right)d^2\sqrt{d-1}}\left\{e^{-\sqrt{(d-1)\mathrm{Pe}}x} + e^{-\sqrt{(d-1)\mathrm{Pe}}(L-x)}\right\} + O\left(\mathrm{Pe}^{-1}\right). \tag{17}$$

Here also, $\chi_R \leq O(1)$ is required for negligible nematic order and the validity of this theory.

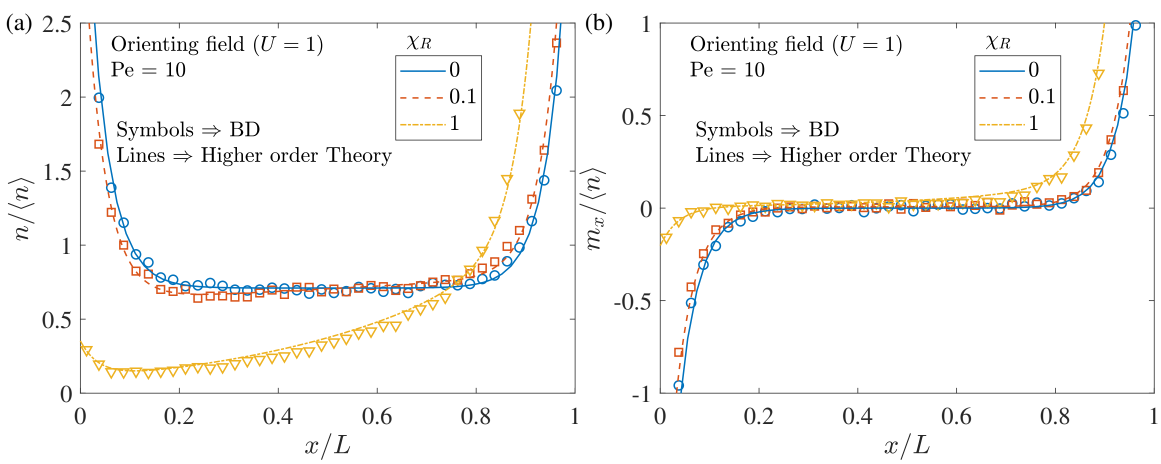

FIG. S1: The number density (a), and the polar order (b) associated with the active matter subjected to the orienting field normal to the walls. The symbols denote the BD simulation results while the lines represent the higher order theory. The confinement region L is 10 times larger than the microscopic length δ.

II. BROWNIAN DYNAMICS SIMULATIONS

The Brownian Dynamics simulations reported in the main text are carried out by numerically integrating over-damped Langevin equations in time [3]

$$\mathbf{0} = -\zeta\dot{\mathbf{x}} + \mathbf{F}^{swim} + \mathbf{F}^{B}, \tag{18}$$

$$\mathbf{0} = -\zeta_R\mathbf{\Omega} + \mathbf{L}^{ext} + \mathbf{L}^{R}, \tag{19}$$

where the particle orientation $\mathbf{q}$ follows $\frac{d\mathbf{q}}{dt} = \mathbf{\Omega} \times \mathbf{q}$. Here ζ, ζ_R, are the the translational and rotational resistances. The swim force $\mathbf{F}^{swim} = \zeta U(\mathbf{x})\,\mathbf{q}$ and the torque exerted by the orienting field $\mathbf{L}^{ext} = \zeta_R \Omega_c (\mathbf{q} \times \mathbf{H})$. The fluctuating force $\mathbf{F}^{B}$ and the torque $\mathbf{L}^{R}$ follow the usual white noise statistics: $\overline{\mathbf{F}^{B}(t)} = \mathbf{0}$, $\overline{\mathbf{F}^{B}(0)\,\mathbf{F}^{B}(t)} = 2k_BT\zeta\delta(t)\,\mathbf{I}$, $\overline{\mathbf{L}^{R}(t)} = \mathbf{0}$, $\overline{\mathbf{L}^{R}(0)\,\mathbf{L}^{R}(t)} = 2\zeta_R^2\delta(t)\,\mathbf{I}/\tau_R$, where the overbar denotes an ensemble average.

The numerical integration of the Langevin equations is carried out using the Euler-Maruyama scheme with the time-step $\Delta t = 10^{-4}\tau_R$ [4]. The simulations are run for 10^5 particles until the time $t = 100\tau_R$. The penetration of particles into the wall is avoided by using the potential-free algorithm [5]. The wall separation L already includes the particle size, and thus the algorithm simplifies to setting the particle position x to 0 or L, respectively, if $x < 0$ or $> L$.

III. NEMATIC ORDER

We also solved the Smoluchowski equation numerically using in-house FEM code. The numerical solution yields the probability density, from which its moments were evaluated. The first two moments, the number density and the polar order, computed are consistent with theory and BD simulations. Typical values of the next moment, nematic order, at various Pe, χ_R and α_L are shown in Fig. S2. Nematic order is small and hence we assume it is safe to neglect for Pe $< 10^3$ and field strengths $\alpha_L < 1, \chi_R < 1$.

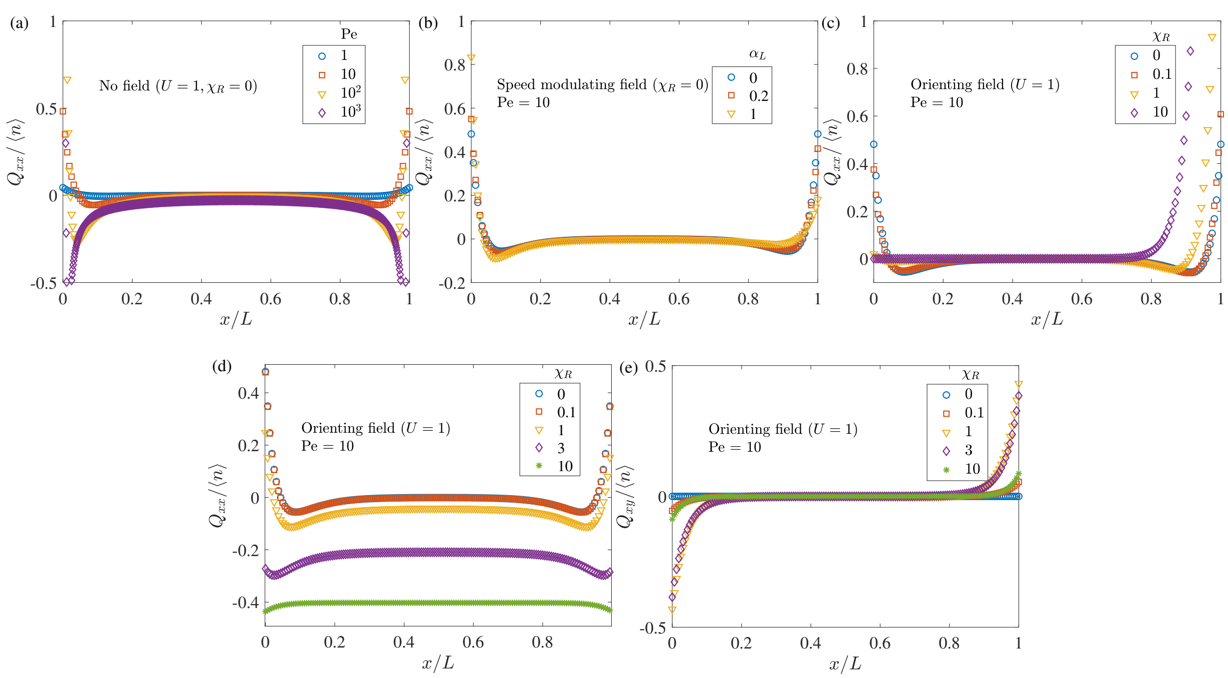

FIG. S2: The nematic order associated with the active matter without any field (a), or subjected to a speed modulating (b) or an orienting field (c) normal to the walls, or an orienting field parallel to the walls (d), (e). The confinement region L is chosen as 10 times larger than the microscopic length δ.

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